

Carbamic acid, ethyl-, methyl ester
6135-31-5 | DTXSID80210261

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.00

Global applicability domain: Inside

Local applicability domain index: 5.52e-01

Confidence level: 6.53e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Methylimidazolidine-2-thione</div> <div>Measured: 10.0</div> <div>Predicted: 4.59</div>	<div>Image not found</div> <div>Paraldehyde</div> <div>Measured: 3.02</div> <div>Predicted: 2.77</div>	<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: 5.01e-01</div> <div>Predicted: 1.06</div>
<div>Image not found</div> <div>2-Isopropyl-6-methyl-4-pyrimidone</div> <div>Measured: 1.82</div> <div>Predicted: 2.23</div>	<div>Image not found</div> <div>N,N-Dimethylformamide</div> <div>Measured: 7.94e-01</div> <div>Predicted: 1.12</div>	